



Multiscale Simulation of Microstructural Evolution in Polycrystalline Materials

D. Wolf

with

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MMM - London, 6/18 - 6/20, 2002



Cluster Supercomputer Using Consumer Electronics

Interfacial Materials Group - Materials Science Division



Hardware

Odin I Beowulf Cluster

36 nodes - 450MHz Pentium III (9/1999)

Upgraded to 1GHz PIII (5/2001)



Odin II Beowulf Cluster

100 nodes - 700MHz Pentium III (8/2000)

Odin III Beowulf Cluster

100 nodes - 2.6GHz Pentium IV (7/2003)

Software

Linux (Red Hat 6.1, Mandrake 7.1)

MPI

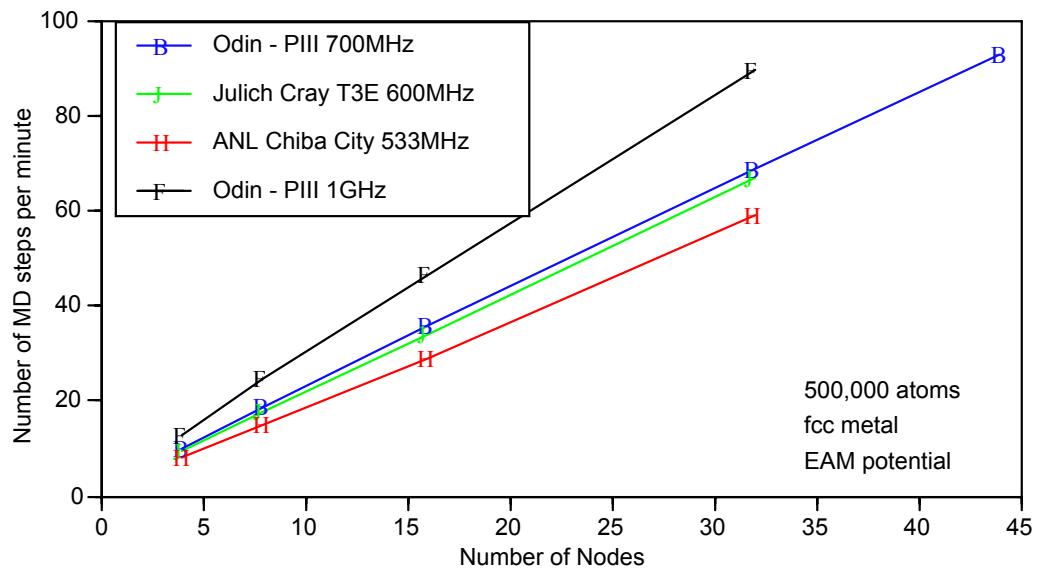
Pentium Group Fortran

Performance

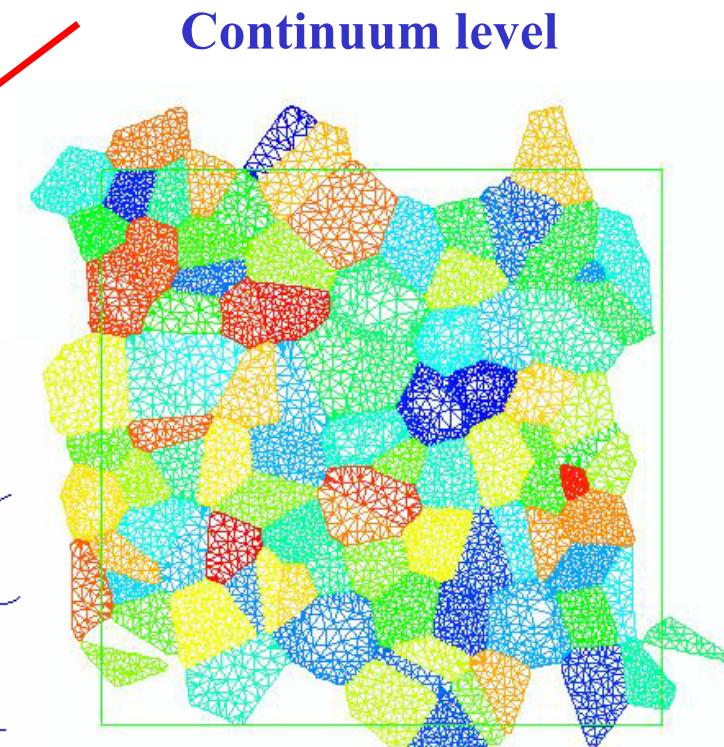
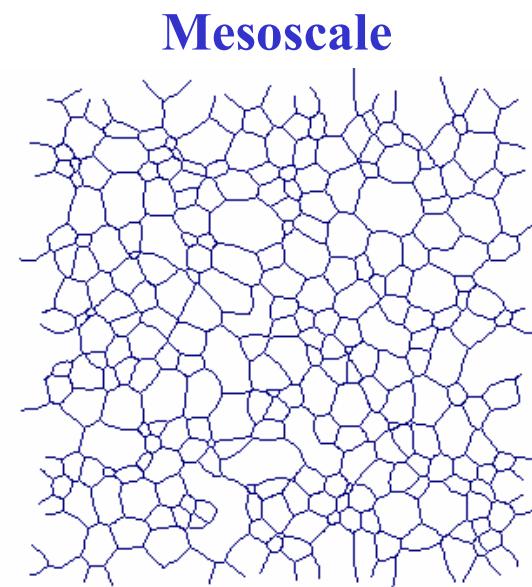
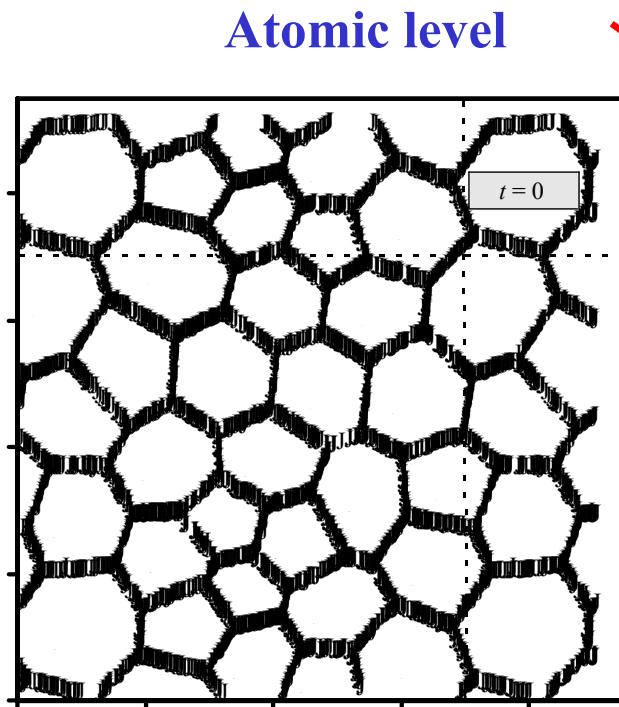
Odin II = Cray T3E 600MHz

Additional information

[www.msd.anl.gov/im/
cluster/odin.html](http://www.msd.anl.gov/im/cluster/odin.html)



Scientific Opportunity: Hierarchical Multiscale Simulation of Microstructural Evolution



Newton's Law

*Principle of virtual-power
dissipation*

*Continuum mechanics,
Constitutive laws*

Goal: *Continuum simulations based on fundamental understanding of GB physics!*

Scientific opportunity

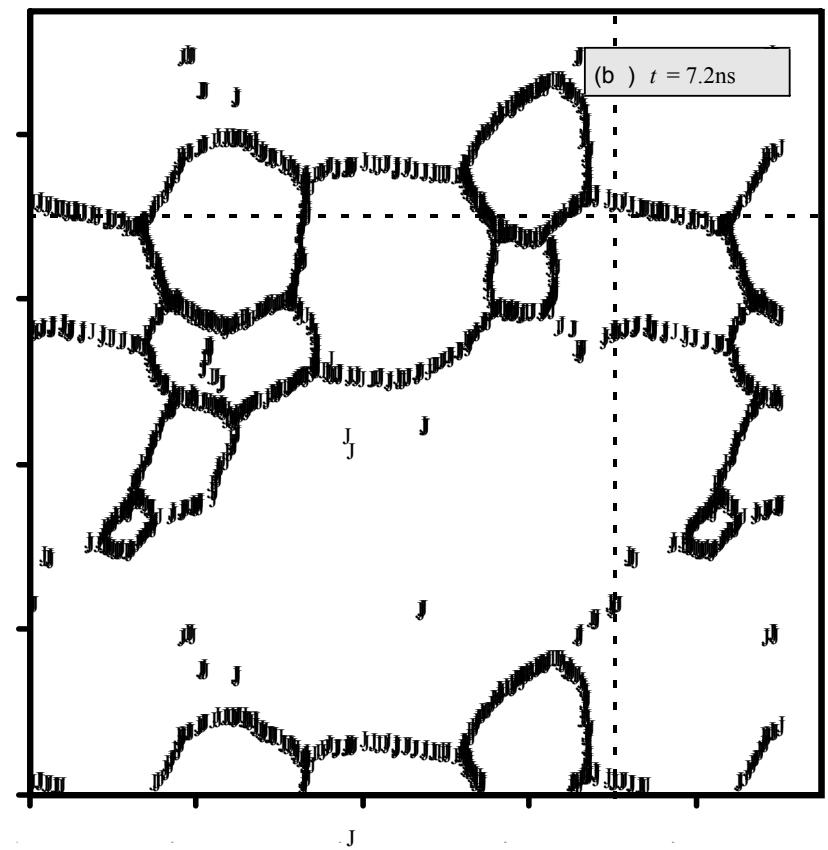
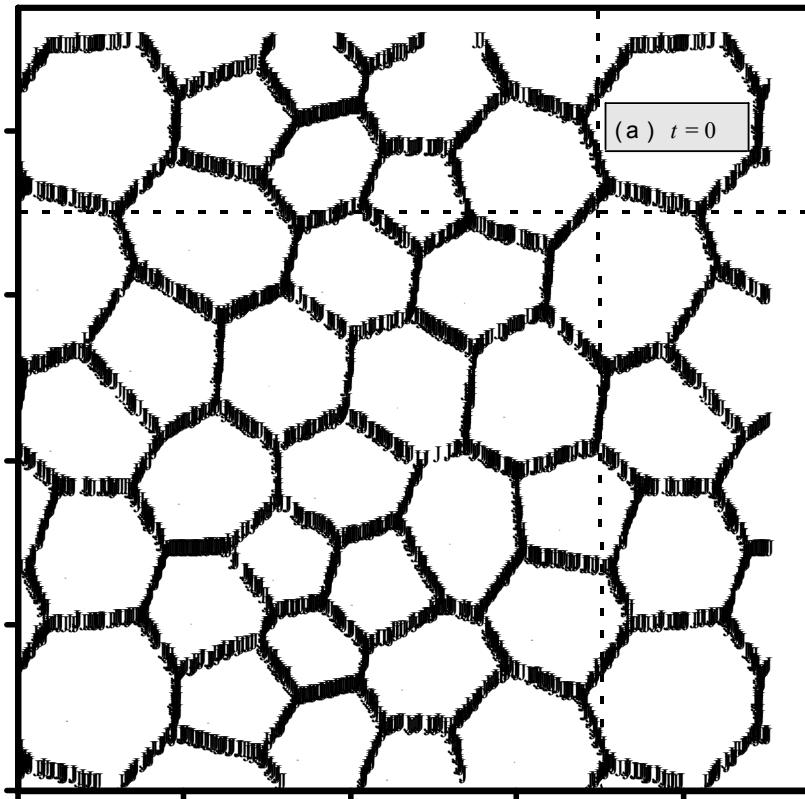
- ‘*Microstructure and deformation physics*’ by *MD simulation*
 - *Dislocation plasticity in nanocrystalline Al*
 - *Grain growth in nanocrystalline Pd*
- *Hierarchical multiscale simulation of polycrystalline materials*
 - *Use grain growth and GB diffusion creep as a case study*
 - *Focus on the atomistic - mesoscale - continuum linkage*

Outline

- MD simulation of grain growth
 - *Identify growth mechanisms*
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 - GB mobility, energy, diffusivity, ...
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Grain growth in a <100> textured Pd polycrystal

(A. Haslam et al., *Mat. Sci & Engin. A* 318, 293, 2001)



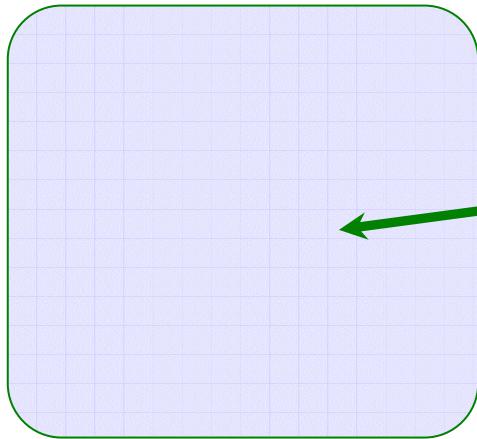
$t=0$

*<100> columnar microstructure
25 grains, $d=15 \text{ nm}$, $\Theta_{\min} \sim 14.9^\circ$,
 $\sim 400,000$ atoms*

$t=7.2 \text{ ns}$

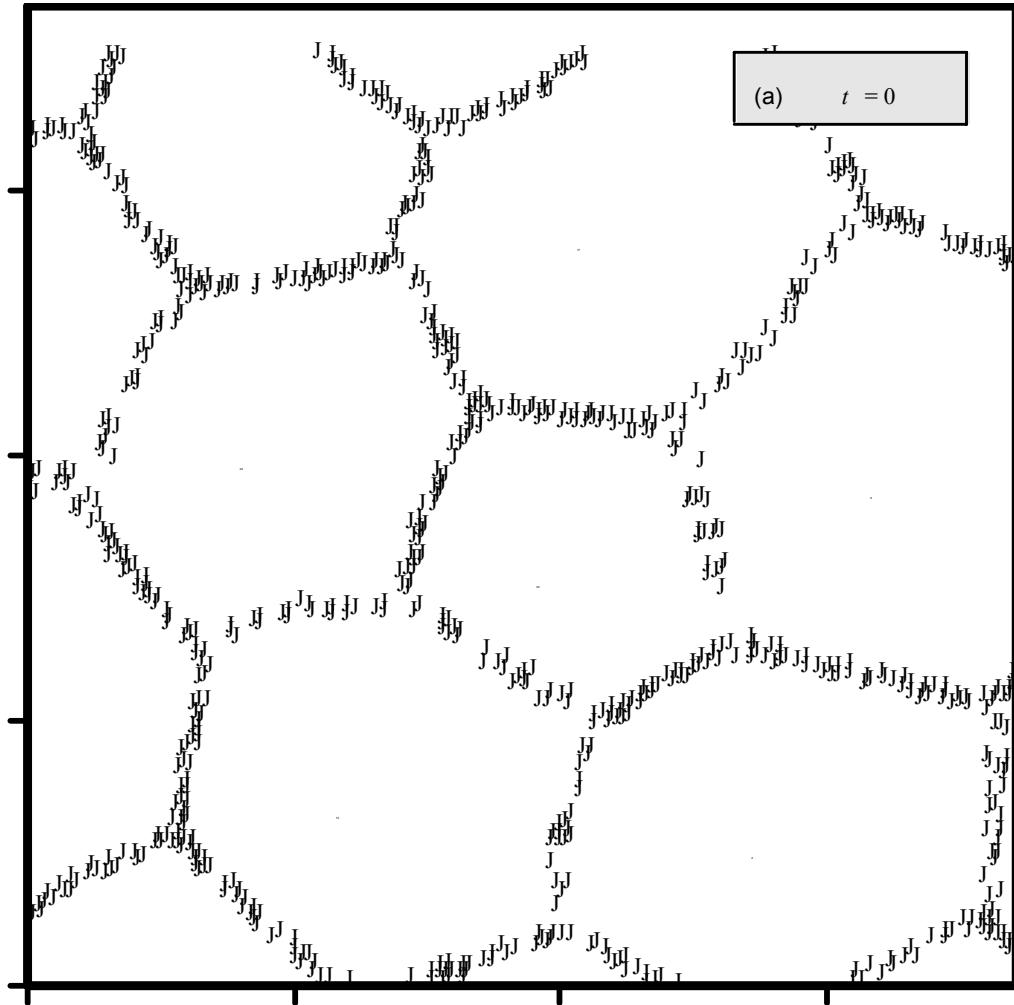
*1.4 million MD time steps
Pd (EAM) potential
fully 3d physics*

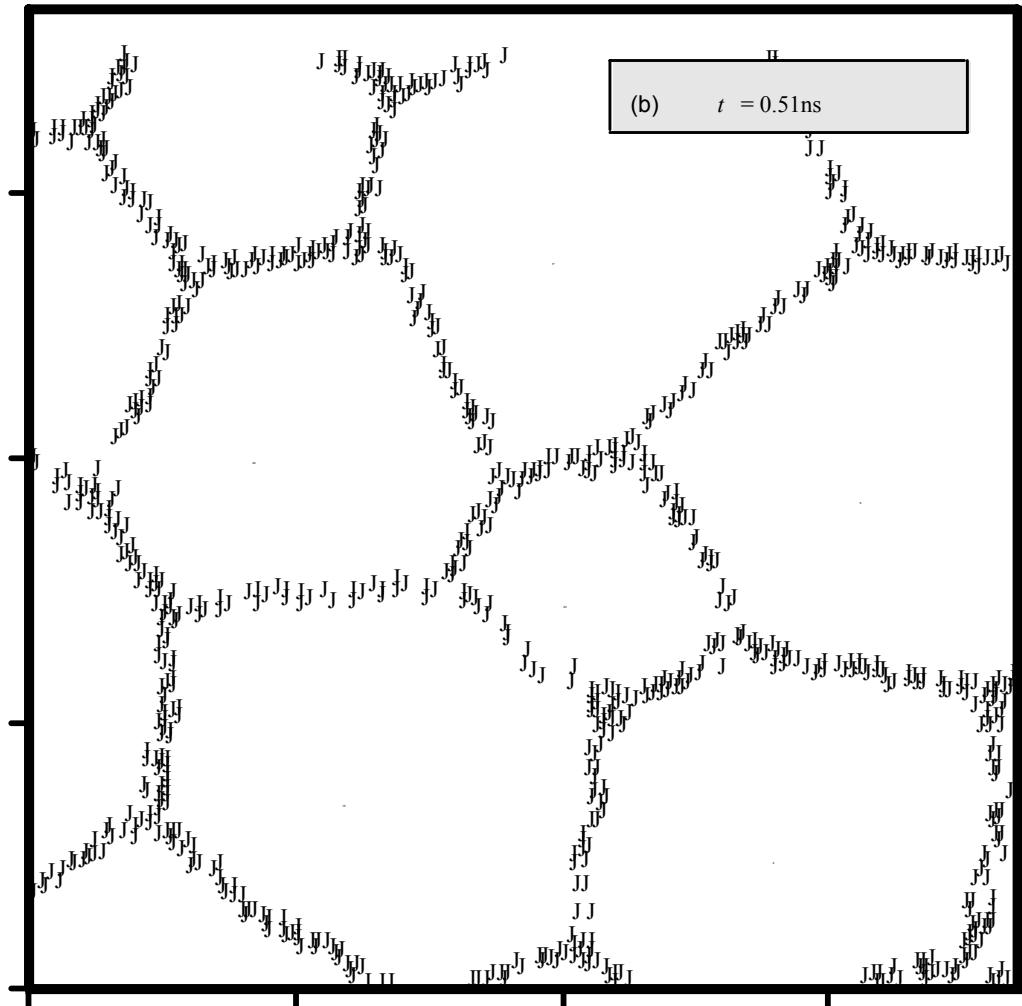
Grain growth on MD time scale (driving force $\sim 1/d$)!

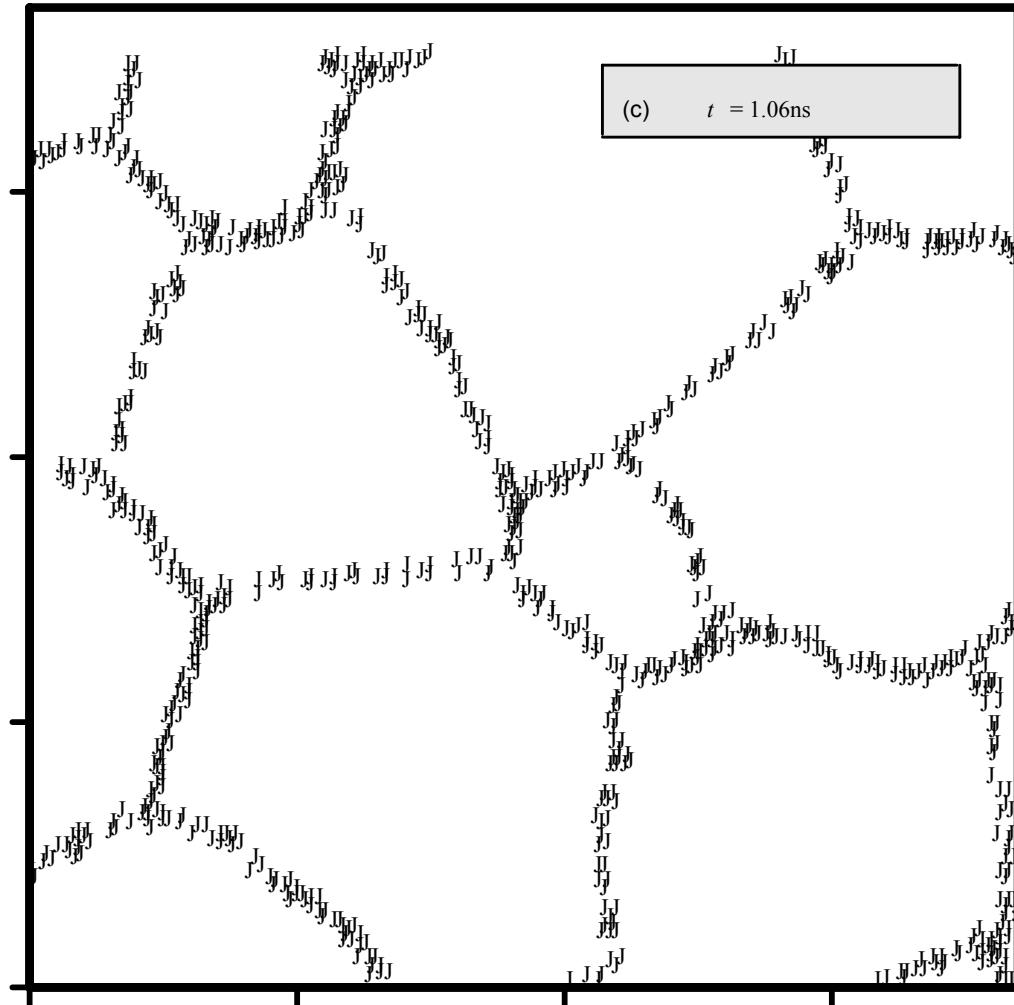


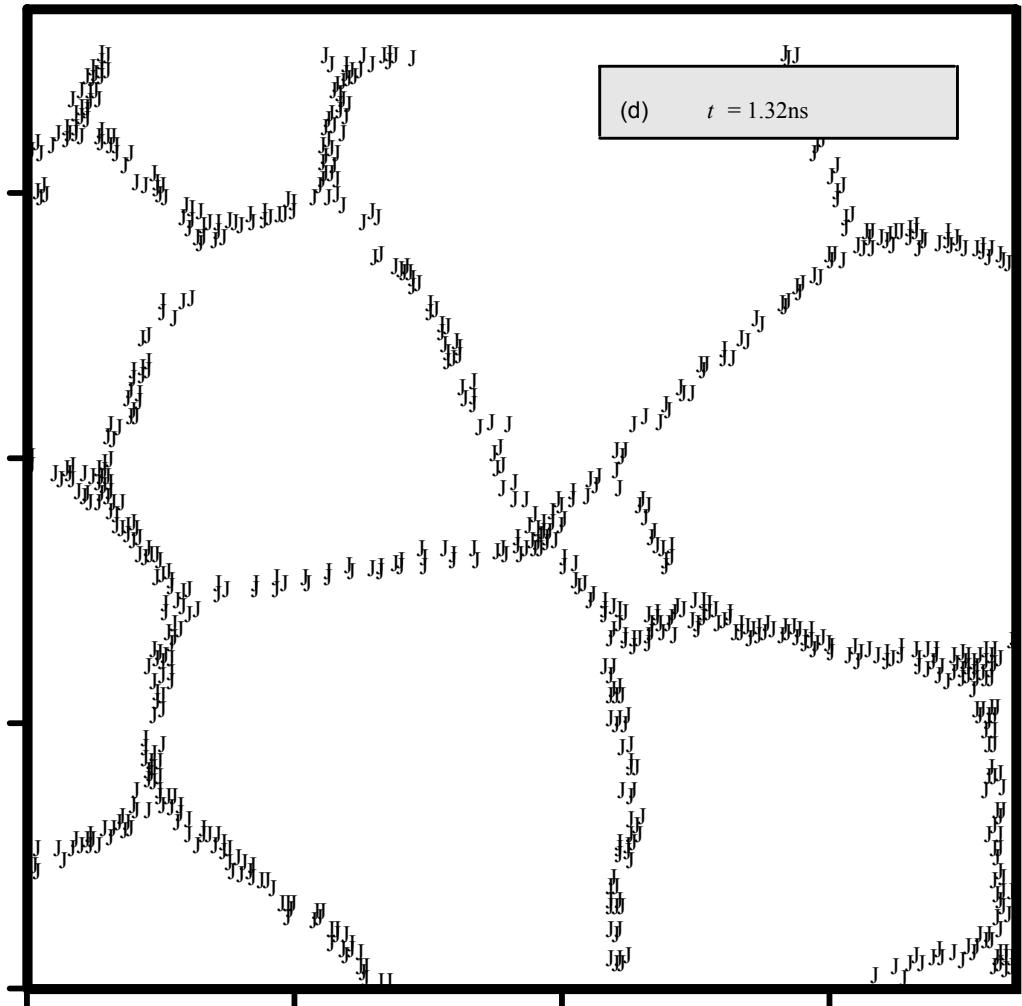
GB migration

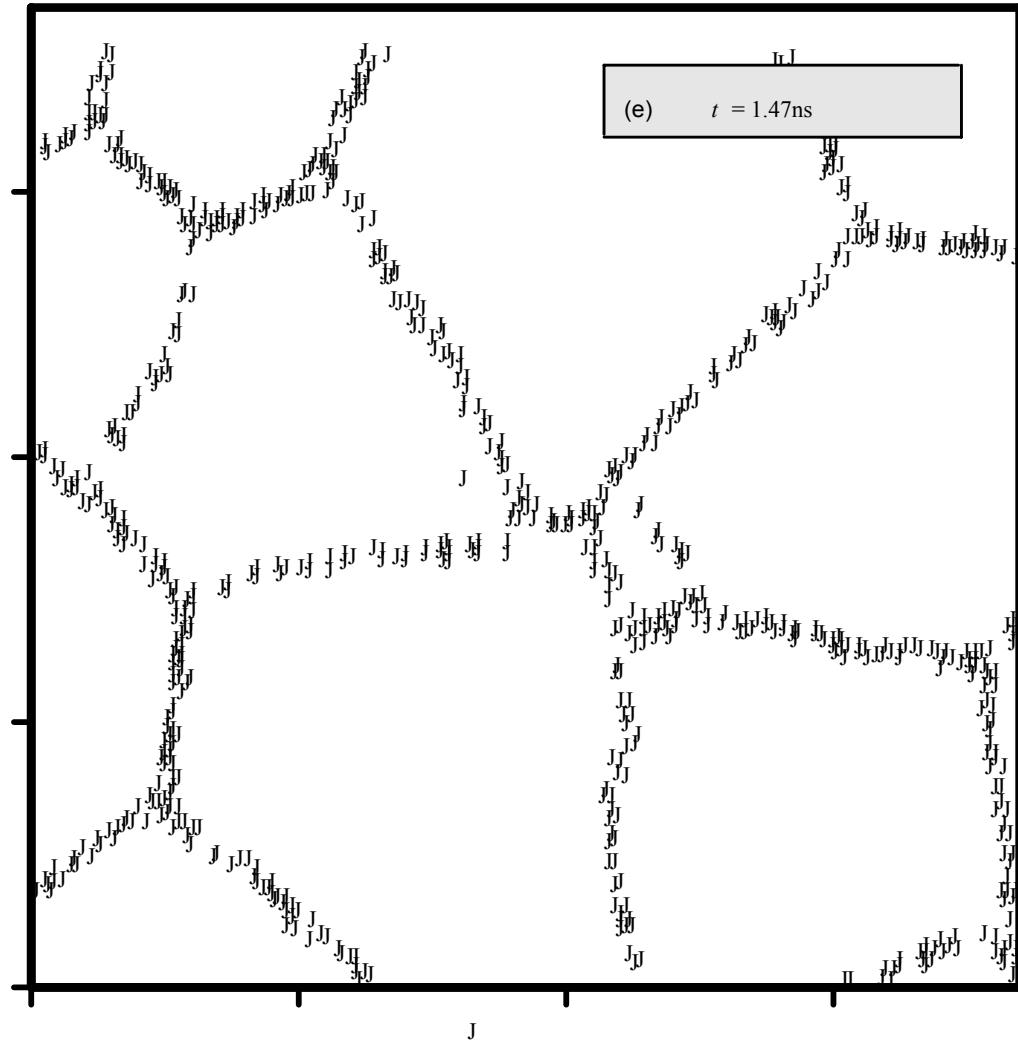
QuickTime™ and a
GIF decompressor
are needed to see this picture.

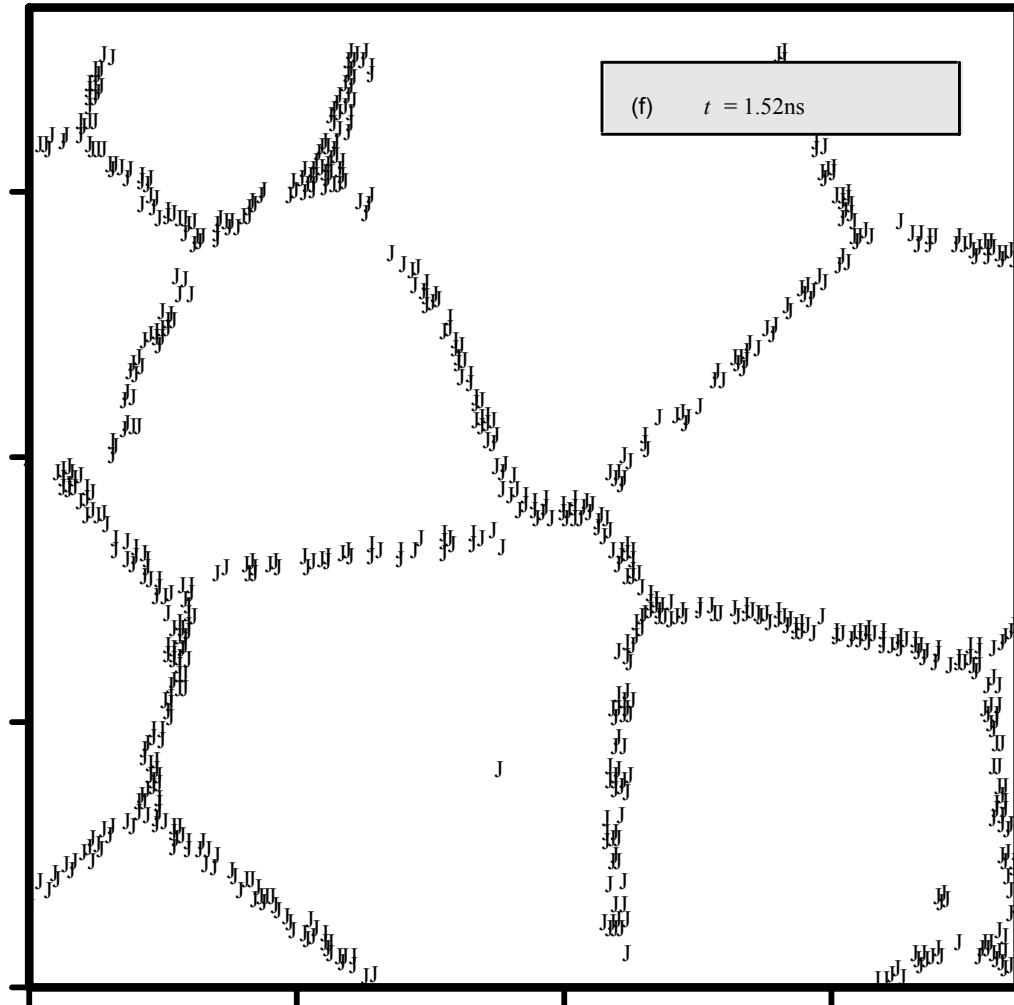






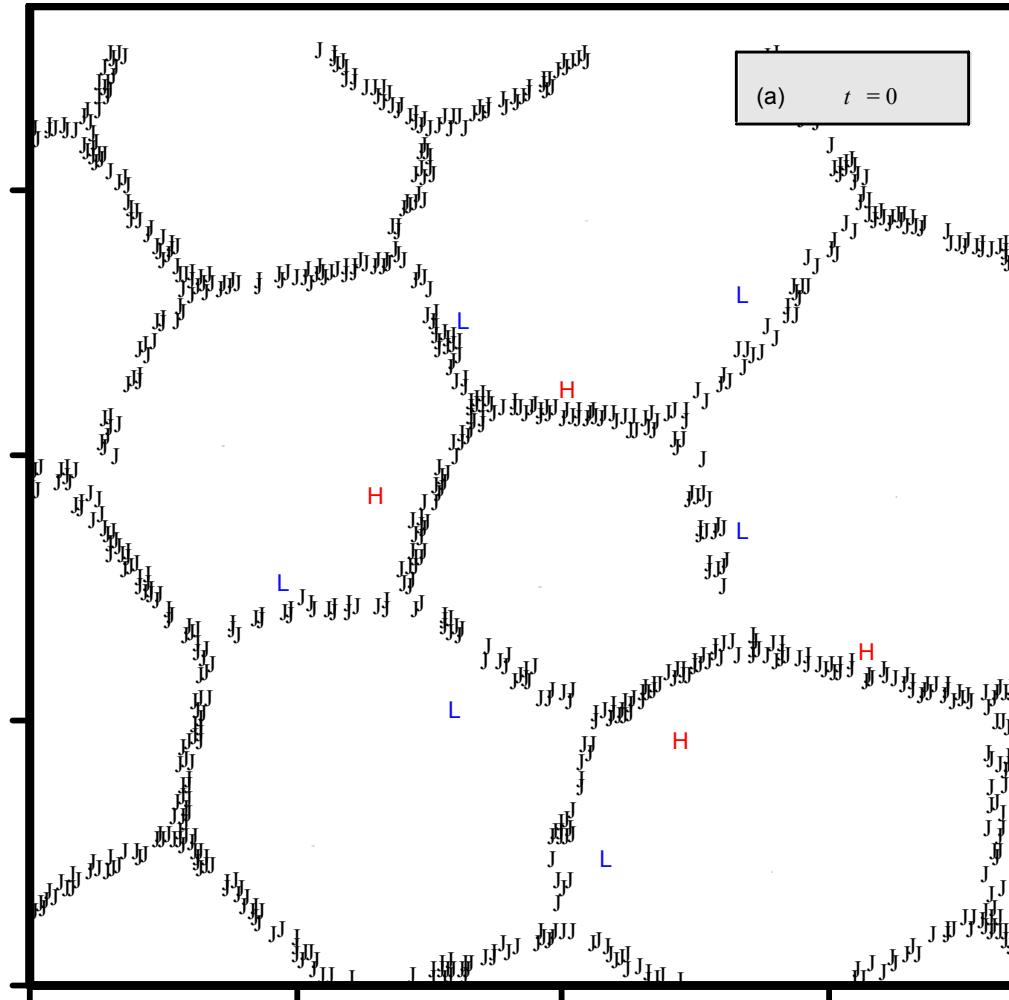




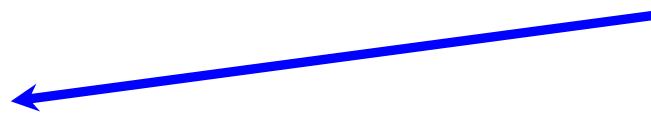
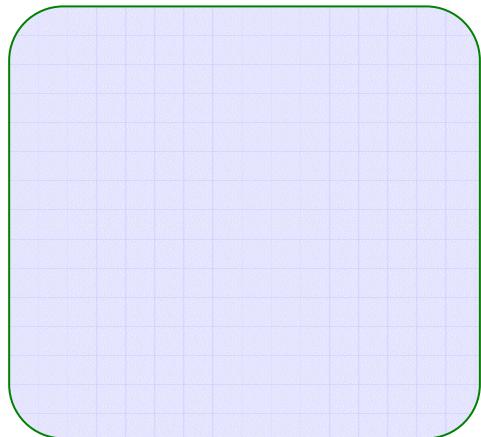


High-energy grain boundaries disappear by GB migration

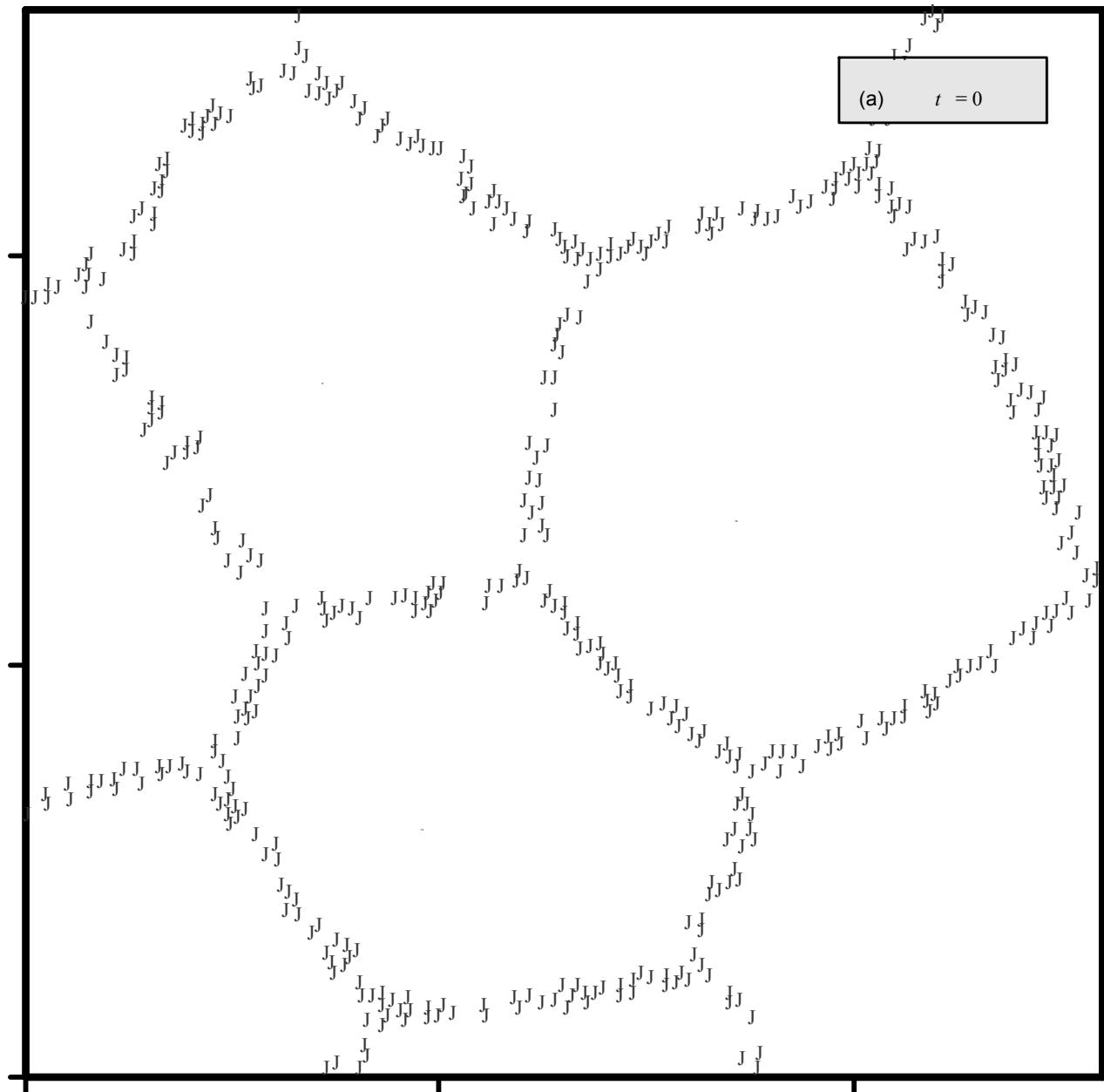
(A. Haslam et al., *Mat. Sci & Engin. A*, 2001)

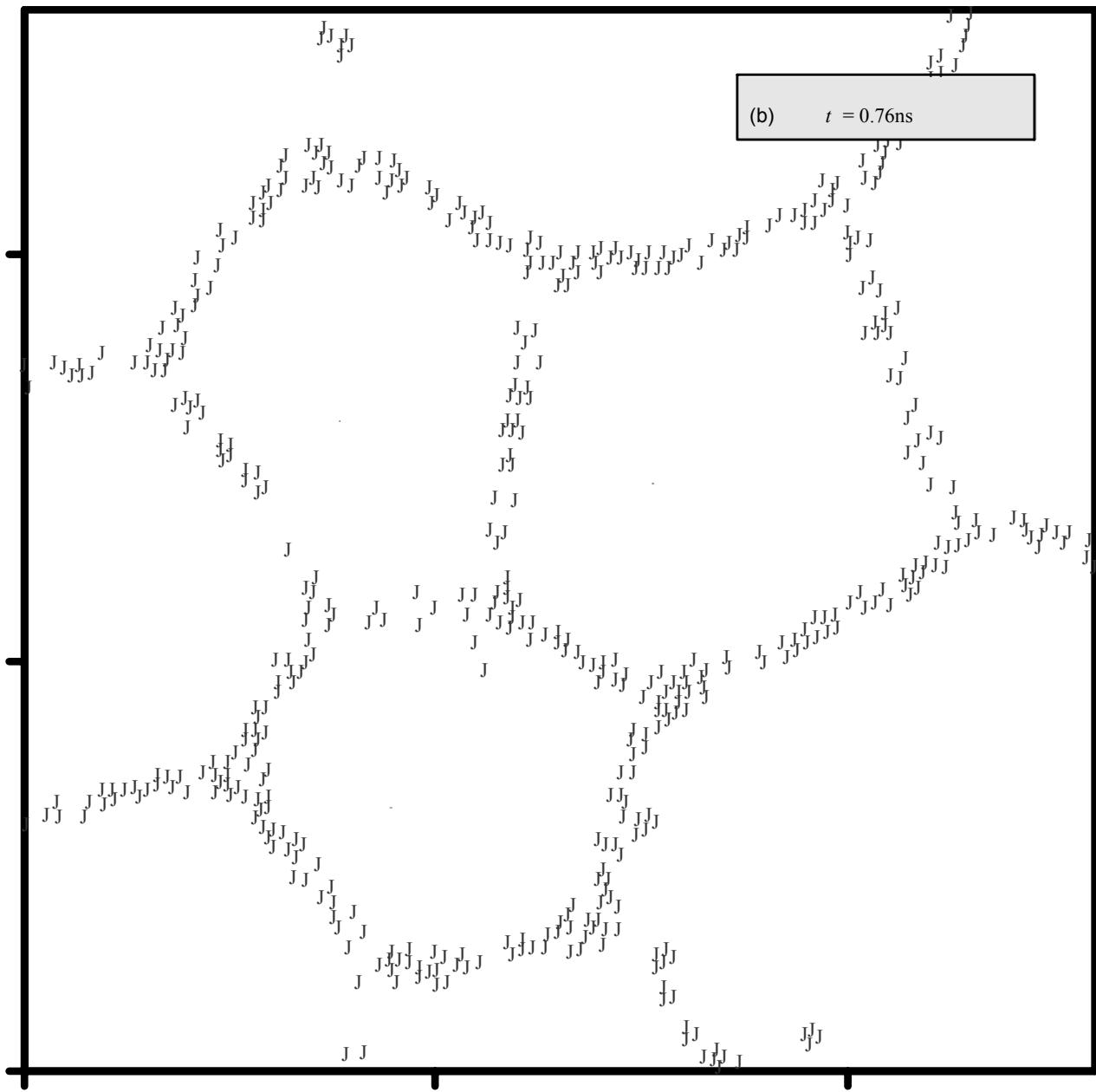


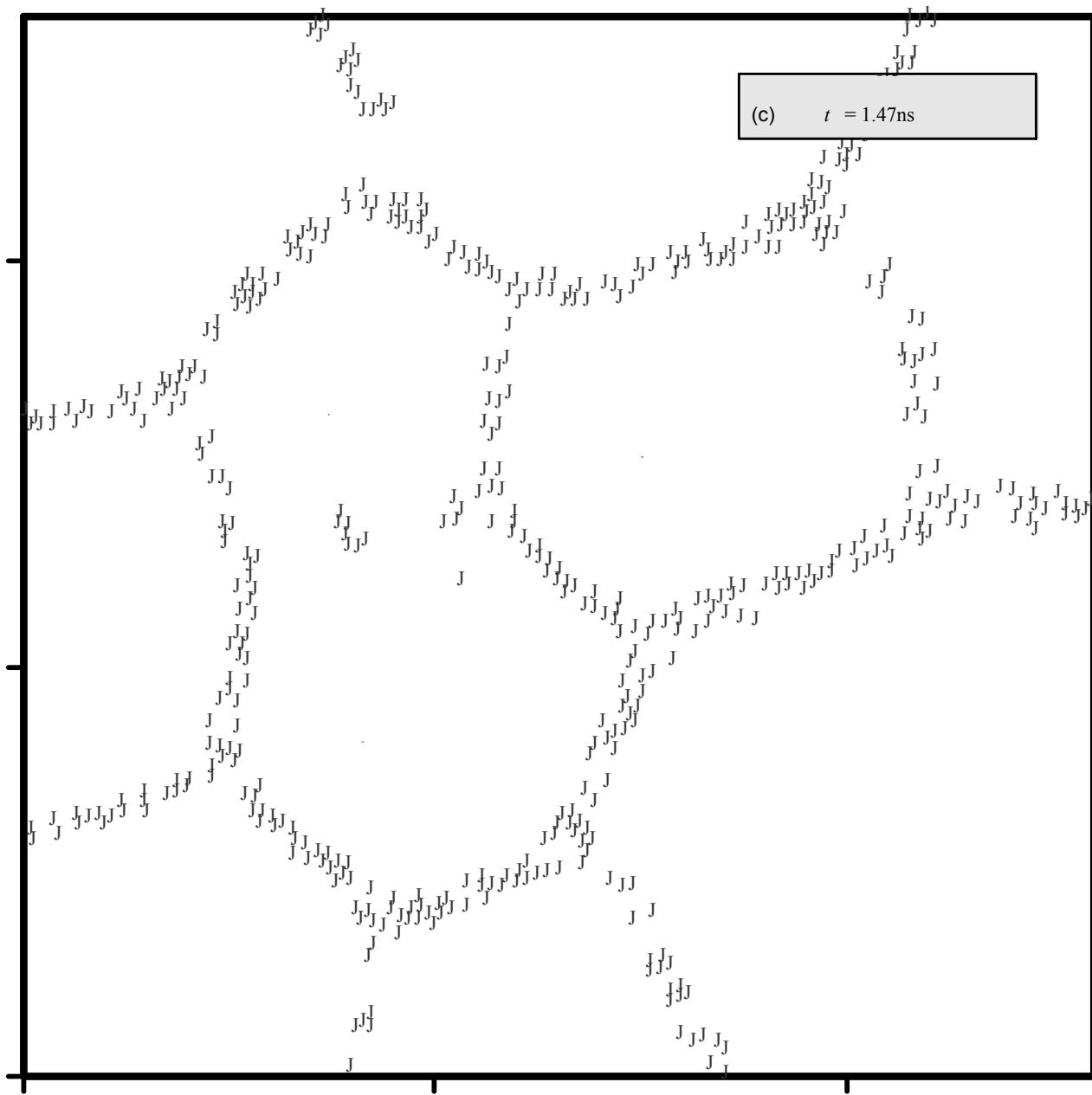
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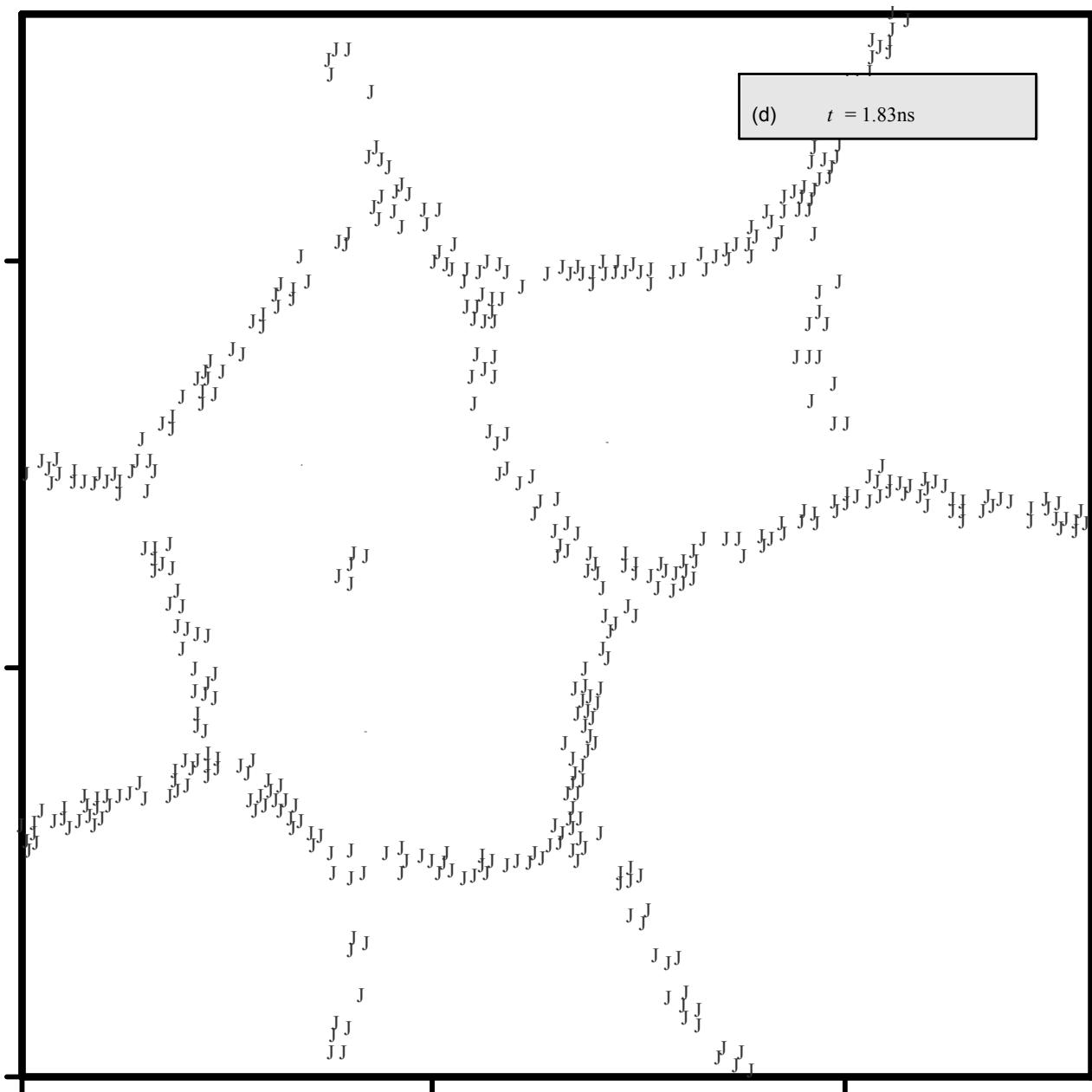
**Grain rotation /
coalescence**

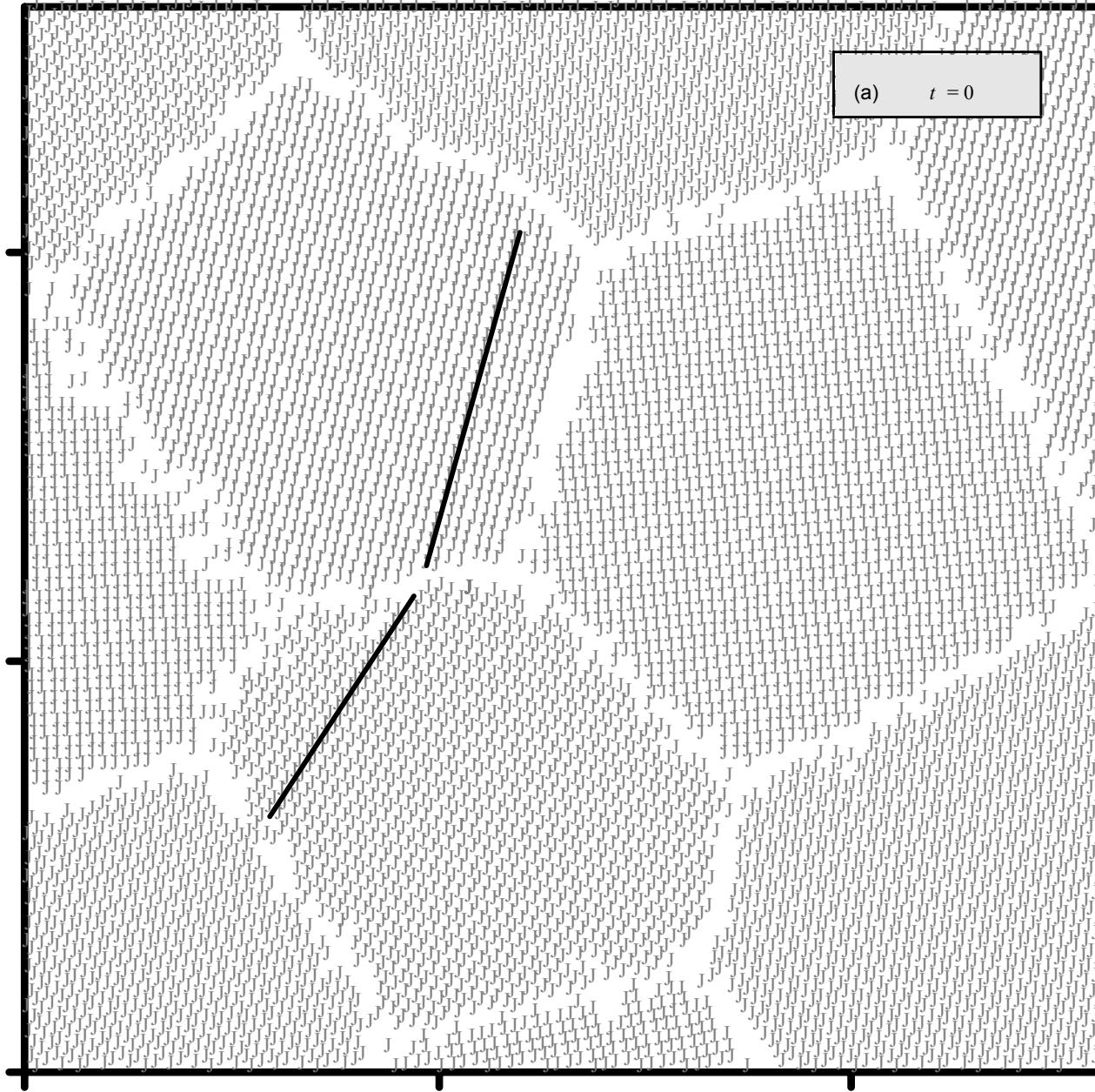




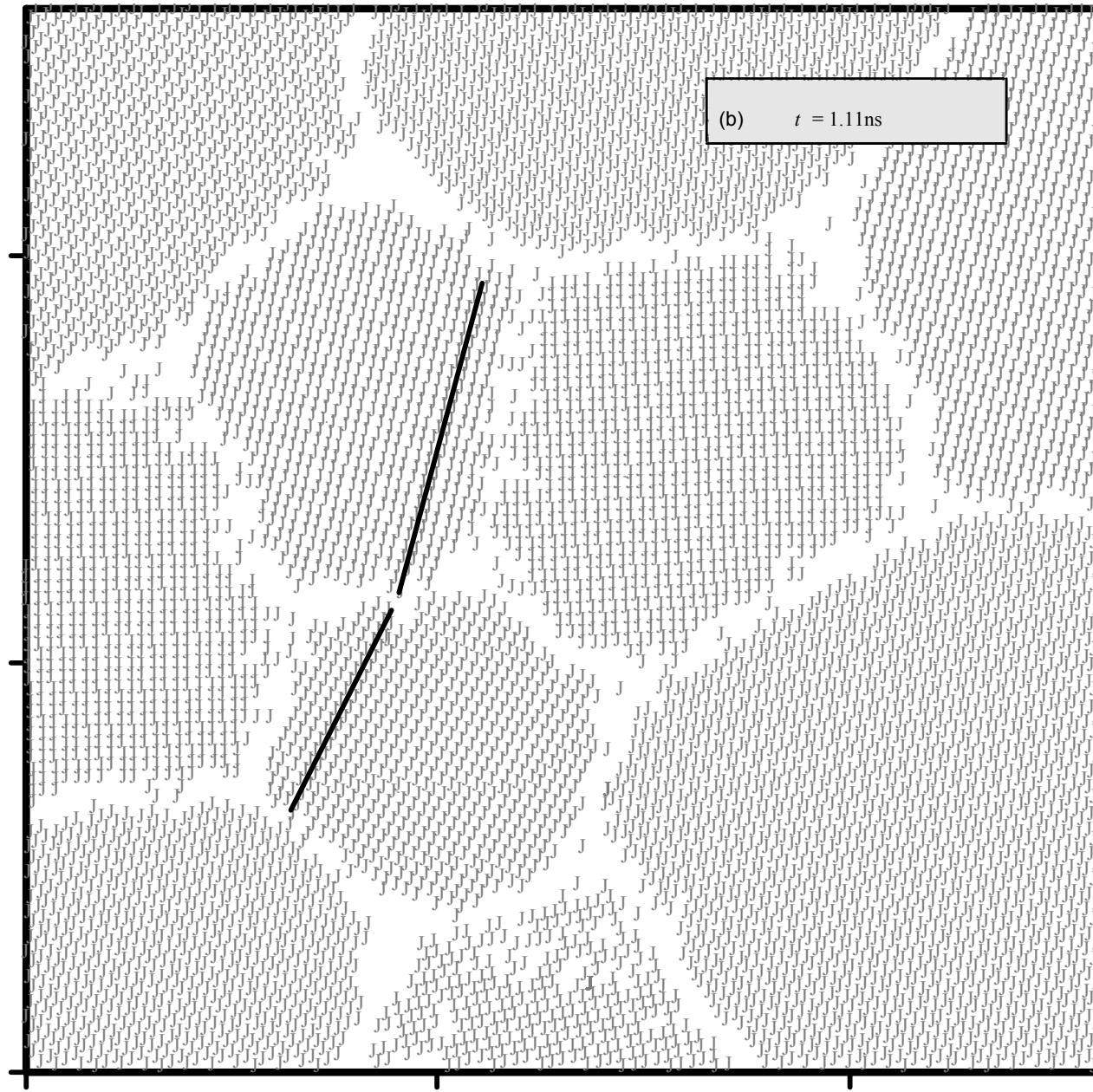


(d) $t = 1.83\text{ns}$

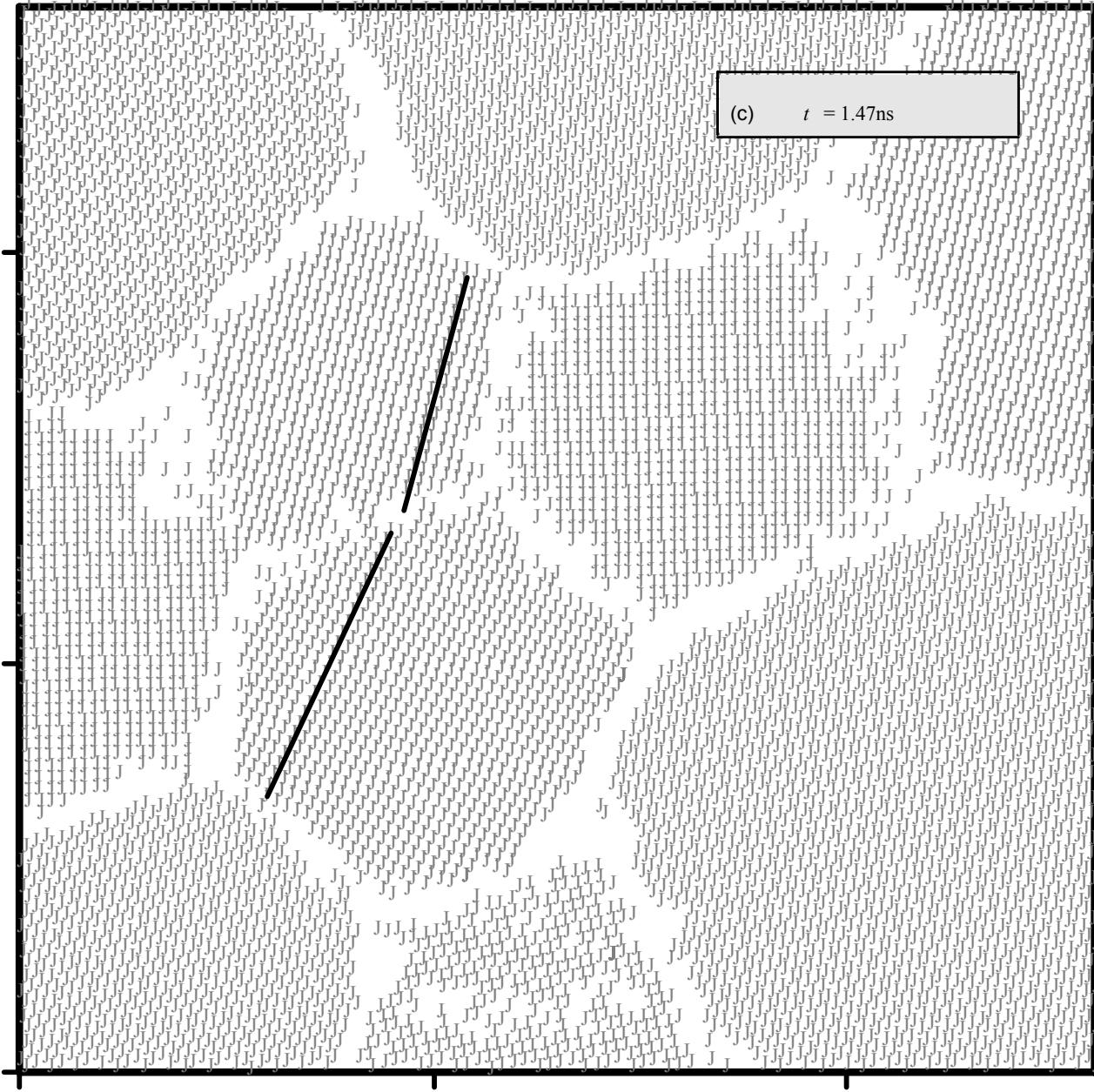




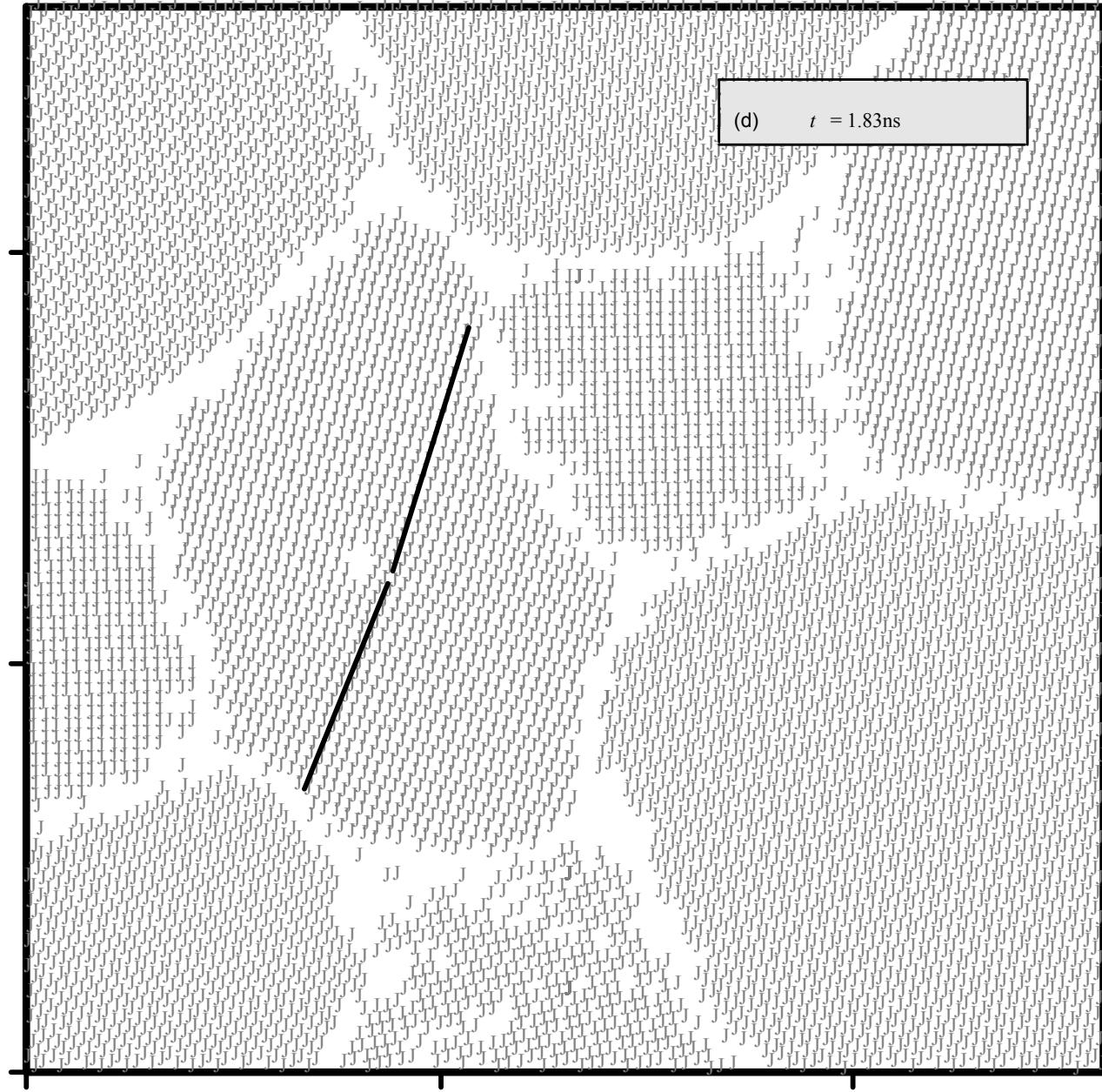
(b) $t = 1.11\text{ns}$



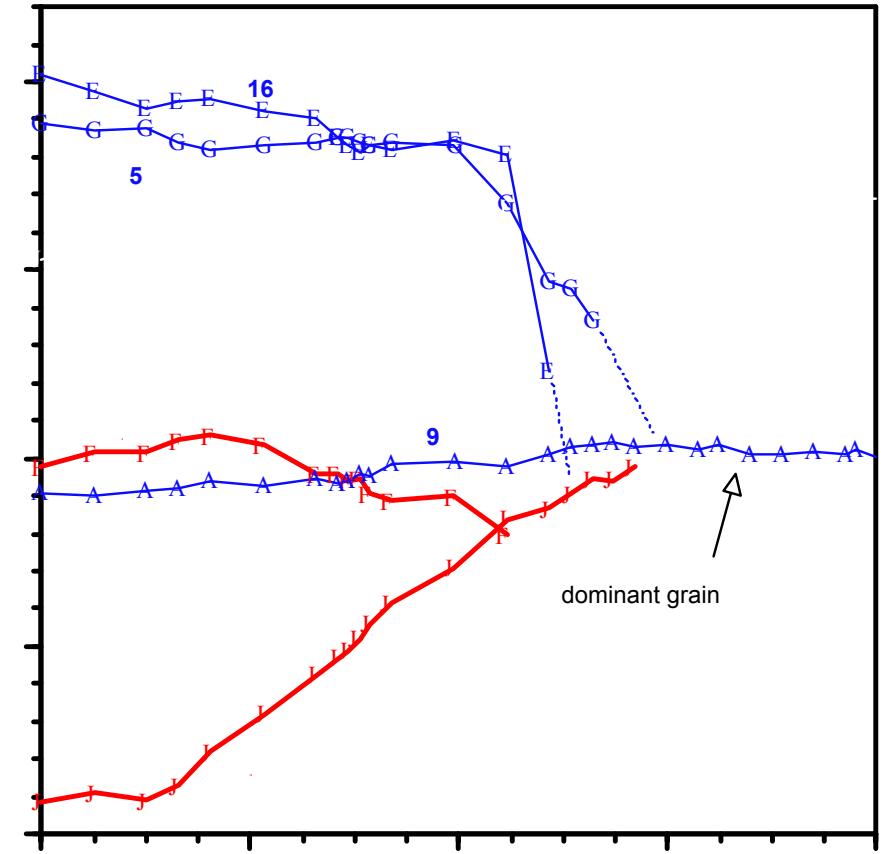
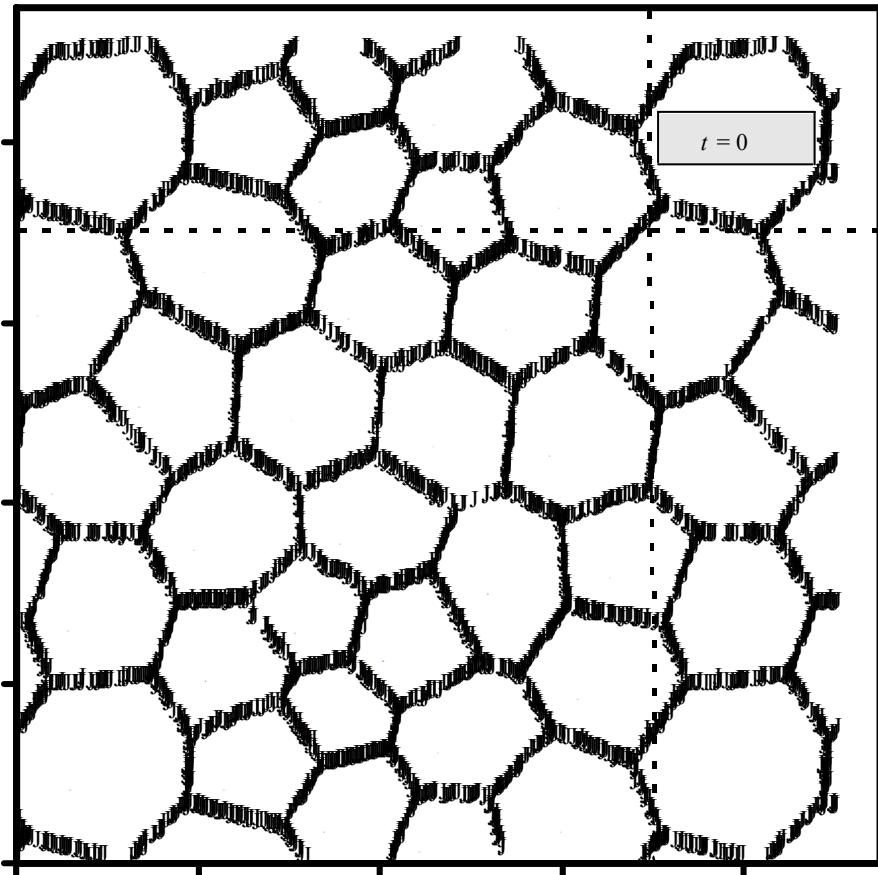
(c) $t = 1.47\text{ns}$



(d) $t = 1.83\text{ns}$



Grain Rotation

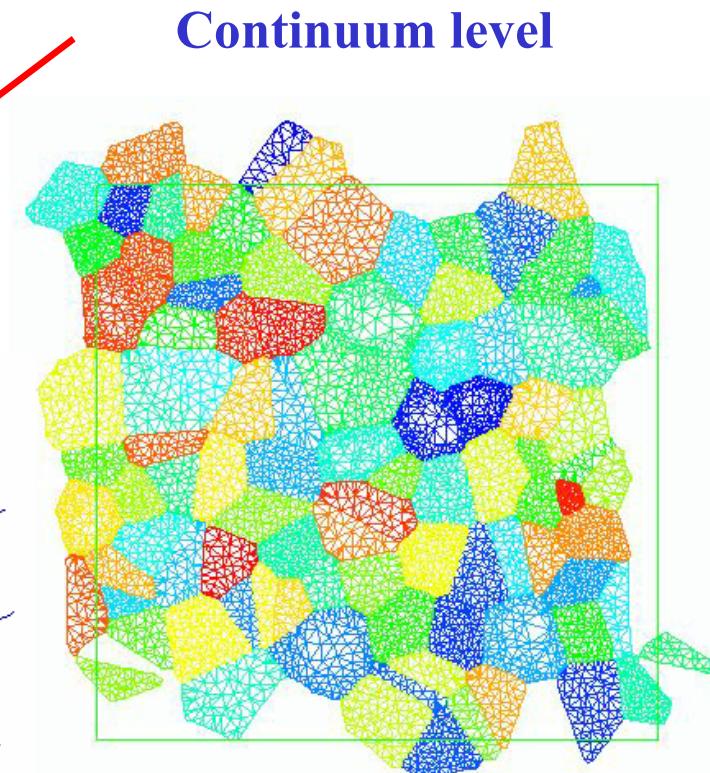
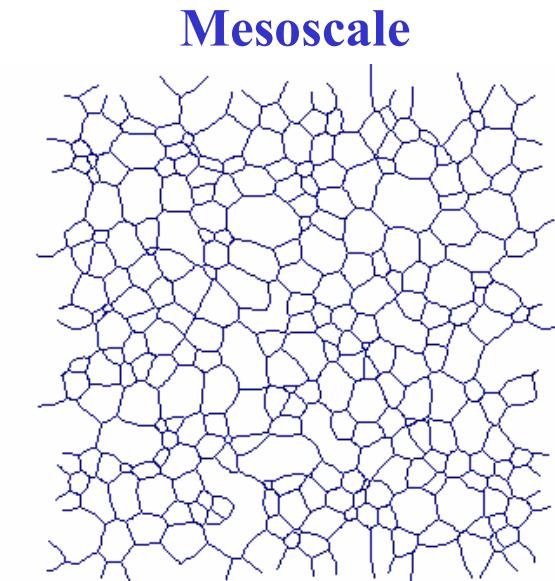
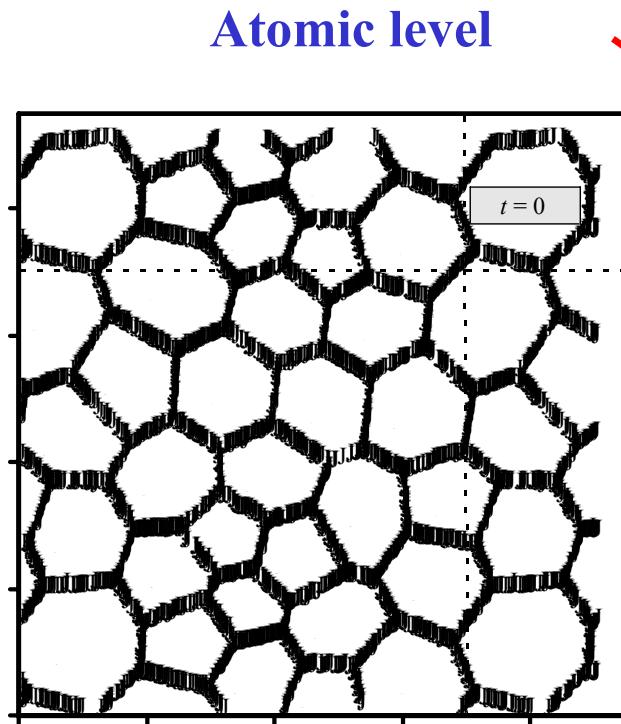


Viscous process: $\omega_i = M_i \tau_i$

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How to transfer atomic-level insights and parameters to the mesoscale?



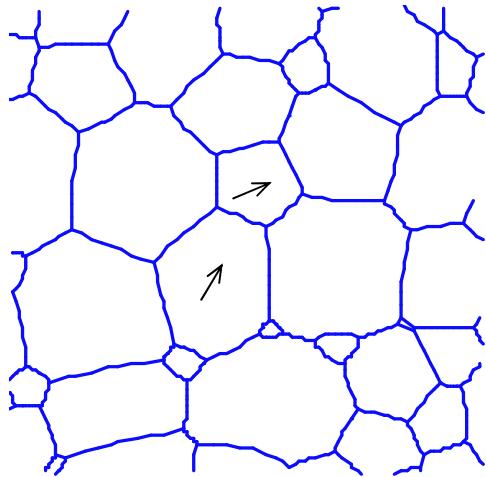
Newton's Law

*Principle of virtual-power
dissipation*

*Continuum mechanics,
Constitutive laws*

Theory of diffusion accommodated grain rotation

(D.Moldovan et. al., *Acta mater.* **49**, 3521, 2001)



$$\omega = M(R) \tau$$

viscous-like rotation

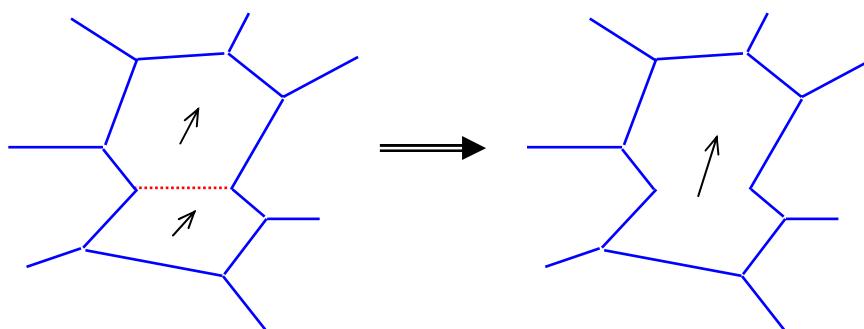
$$\tau = \sum_{k=1}^{Nsides} L_k \left(\frac{d\gamma}{d\theta} \right)_k$$

“cumulative torque”

$$M(R) = \frac{A(\Omega, \delta D_{GB}, T, shape)}{R^5}$$

diffusion accommodated

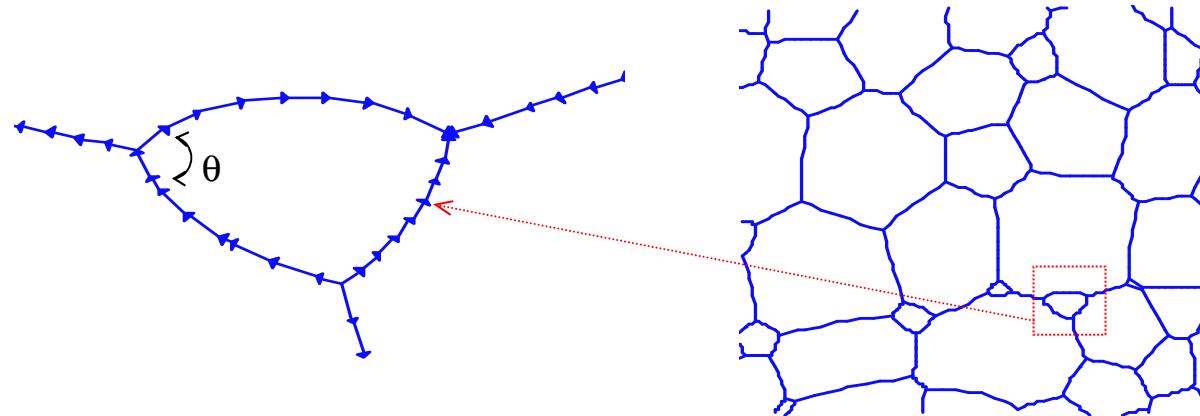
Grain coalescence by grain rotation



Mesoscale Simulations (2d)

(D. Moldovan et. al., *Phil. Mag. A* 82, 1271, 2002)

- Discretized GBs:



- Variational functional for dissipated power (Needleman & Rice 1980, Cocks 1992, see also Ziegler, *Introduction to Thermomechanics*, 1977):

$$\Pi_m(v; k, \gamma, \mu) \quad \Pi_r(\omega; \tau, M)$$

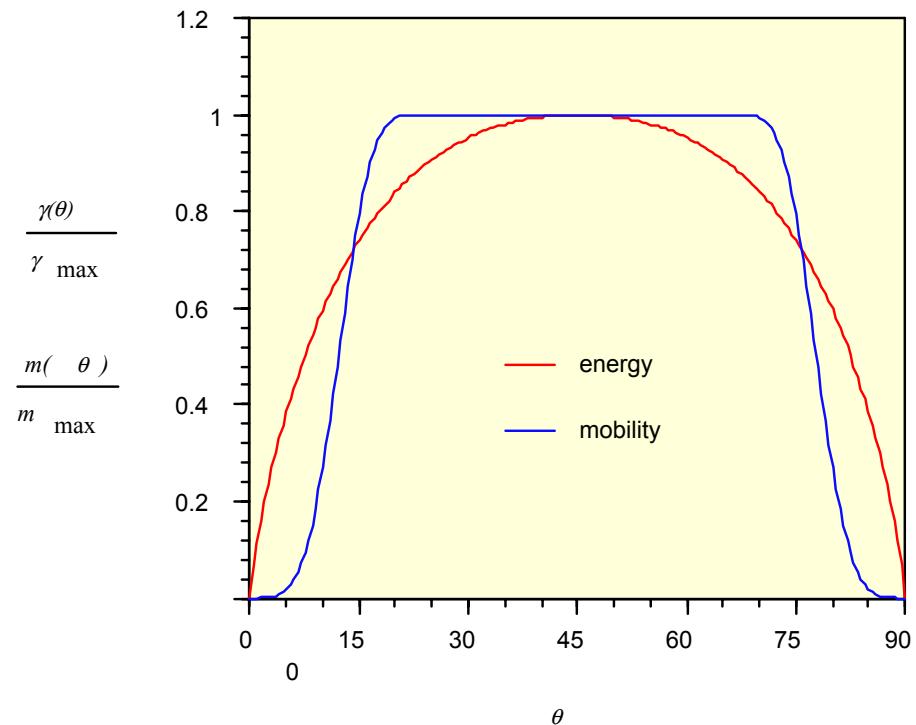
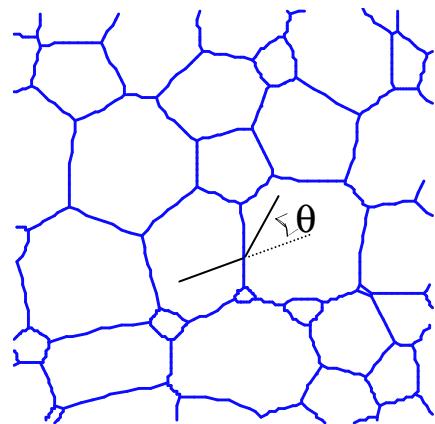
GB velocity *Angular velocity* *GB mobility* *Rotational mobility*
 Local GB curvature *GB energy* *Torque*

- Viscous force laws: *Replace Newton's law! Terms are additive!*

$$v = \mu \gamma / r ; \quad \omega_i = M_i \tau_i ; \quad M_i \sim d^{-5} ; \quad \omega_i \sim d^{-4} ; \quad (\text{D. Moldovan et al., } \textit{Acta mater.} 49, 3521 2001)$$

- Velocity Monte-Carlo or FEM Simulation (F. Cleri, *Physica* 282, 339, 2000; Cocks, 1992)
- Triple-point equilibrium condition (Herring relation) not enforced *a priori*.

Anisotropic grain-boundary properties ; <001> tilt boundaries



$$\frac{\gamma(\theta)}{\gamma_{\max}} = \sin(2\theta) \left[1 - \frac{E_s}{E_c} \ln(\sin(2\theta)) \right]$$

(Extended Read-Shockley; Wolf 1989)

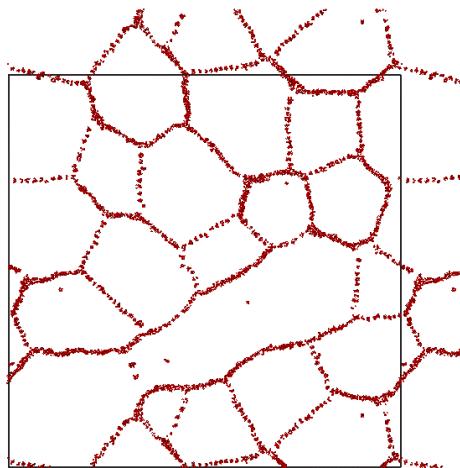
$$\frac{m(\theta)}{m_{\max}} = 1 - \exp\left[-B\left(\frac{\theta}{\theta_0}\right)^n\right]$$

(Humphreys, 1995)

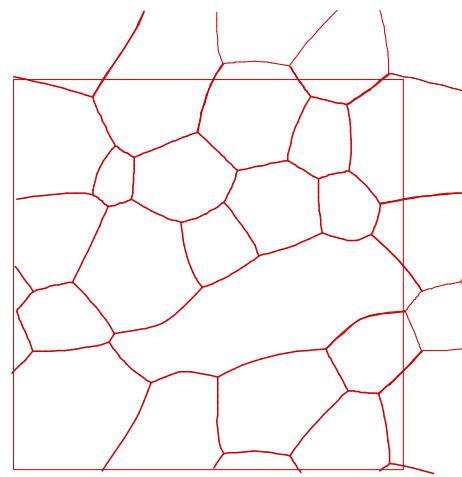
Validation of mesoscale approach against MD simulations

(D. Moldovan et al., *Phil. Mag.* 83, 3643, 2003)

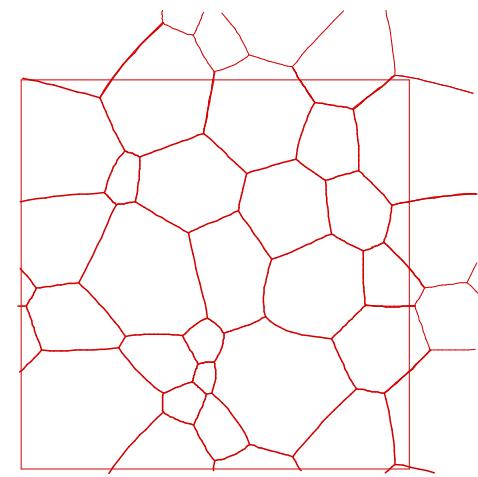
MD: t = 2.89 ns



meso *with* grain
rots.: t = 2.47 ns



meso *without* grain
rots.: t = 2.64 ns



Newton's laws for atoms

Dissipative dynamics for GBs based on virtual power dissipation

- *Distinct processes enter as additive terms in the power functional: dislocations, GBs, ...*
- *Ability to deconvolute interplay between distinct processes and driving forces!*

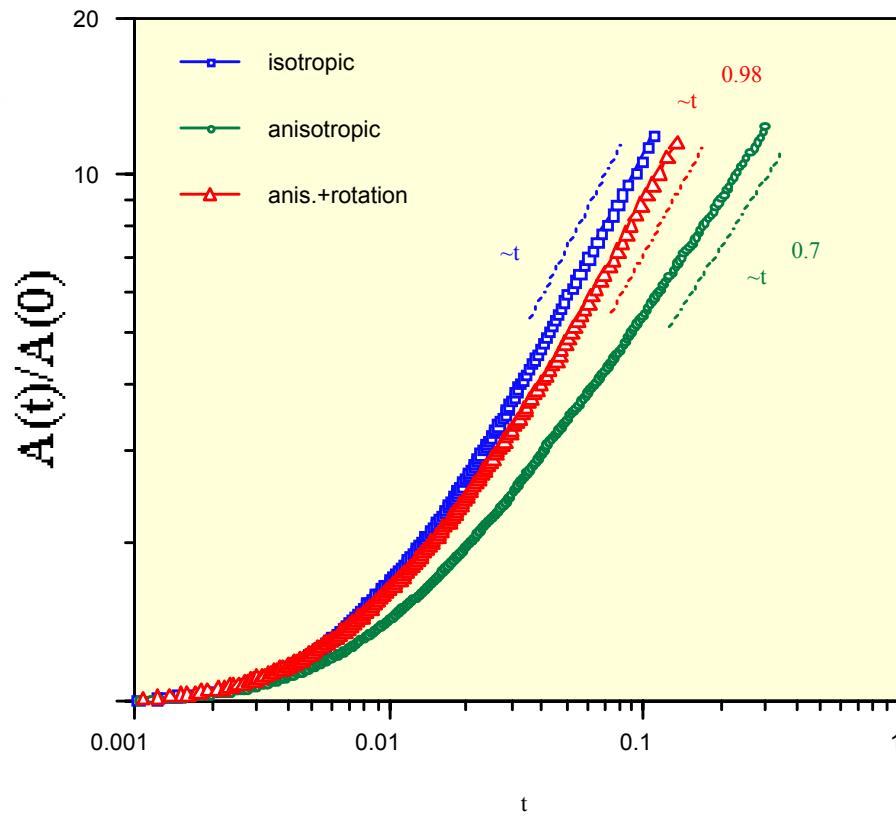
QuickTime™ and a
GIF decompressor
are needed to see this picture.

No grain rotation



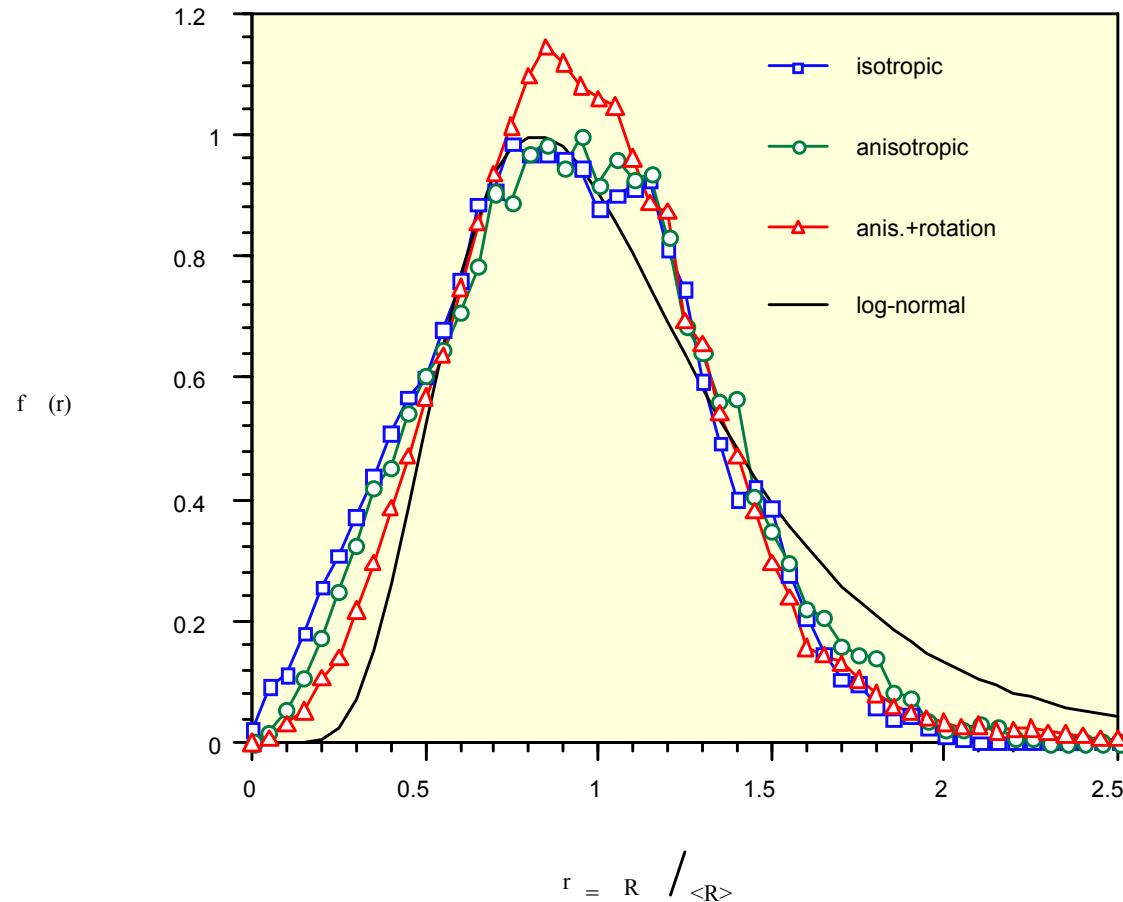
With grain rotation

Growth law



- Asymptotic power law at large times: $A(t) \sim t^\alpha$
 - isotropic $\alpha = 1.00 \pm 0.02$
 - anisotropic $\alpha = 0.70 \pm 0.02$
 - anisotropic+grain rotation: $\alpha = 0.98 \pm 0.02$

Grain size distribution function



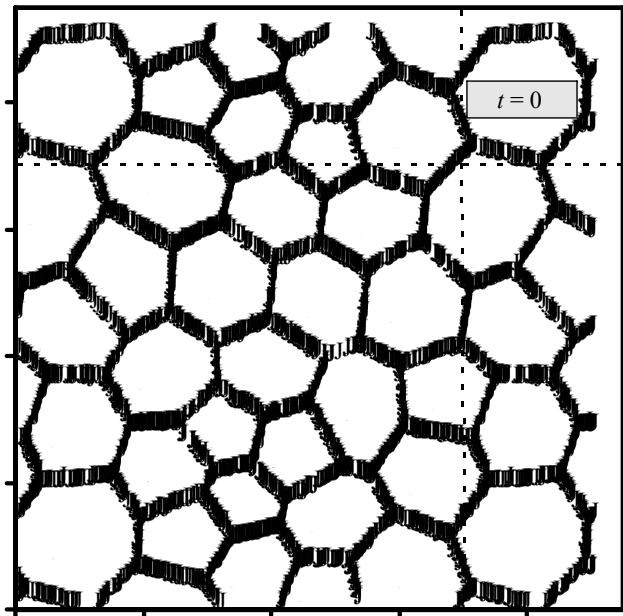
- Rotation leads to a narrower grain-size distribution function

Outline

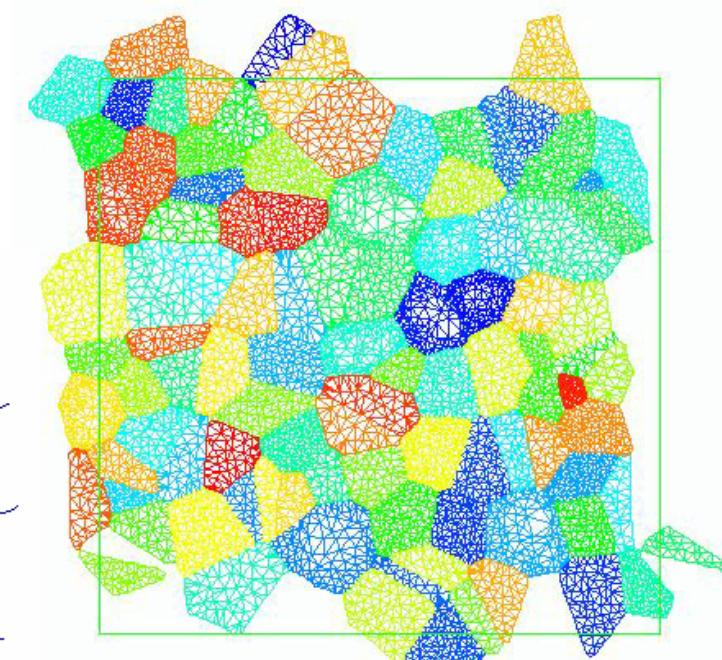
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Effects of Stress: connection with continuum level

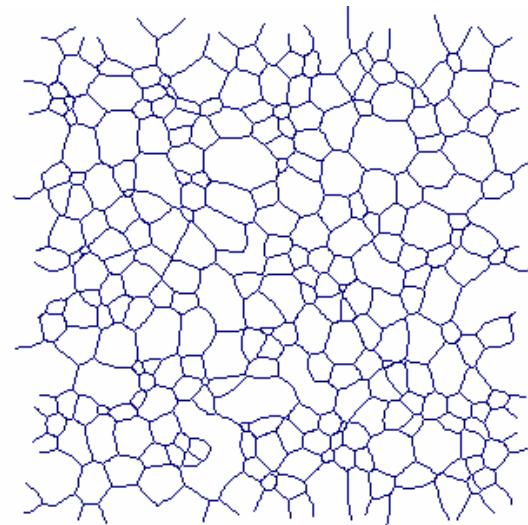
Atomic level



Continuum level



Mesoscale



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Ultimate goal: *Dynamical FEM-type mesoscale simulations with input based on fundamental understanding of the structure and properties of the microstructural elements*